Enhancement of Pairing Correlation by t' in the Two-Dimensional Extended $t-J$ Model

C. T. Shih[1], T. K. Lee[2], R. Eder[3], C.-Y. Mou[4] and Y. C. Chen[1]
[1]*Department of Physics, Tunghai University, Taichung, Taiwan*
[2]*Institute of Physics, Academia Sinica, Nankang, Taiwan*
[3]*Institut für Festkörperphysik, Forschungszentrum Karlsruhe, Germany*
[4]*Department of Physics, National Tsing Hua University, Hsinchu, Taiwan*
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We investigate the effects of the next-nearest-neighbor (t') and the third-nearest-neighbor (t'') hopping terms on superconductivity correlation in the 2D hole-doped extended $t-J$ model based on the variational Monte-Carlo, mean-field calculation, and exact diagonalization method. Despite of the diversity of the methods employed, the results all point to a consistent conclusion: While the $d-$wave SC correlation is slightly suppressed by t' and t'' in underdoped regions, it is greatly enhanced in the optimal and overdoped regions. The optimal T_c is a result upon balance of these two opposite trends.

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Right after the discovery of high temperature superconductors, the two-dimensional (2D) $t-J$ model has been proposed to provide the mechanism of superconductivity (SC)[1]. This idea quickly gained momentum when variational calculations showed that the doping dependence of pairing correlation[2, 3] and the phase diagram of antiferromagnetic (AFM) phase and SC [4] seem to agree with experimental results fairly well. However, recently calculations[5] beyond the variational method have challenged the notion that pure 2D $t-J$ model without including other interactions is enough to explain the high values of T_c. Although this issue is yet to be settled[6, 7, 8], there are results by band-structure calculations[9, 10] and experimental analysis[11] that hopping beyond nearest neighbors is essential to raise T_c. In fact they found highest $T_{c,max}$ for different monolayer cuprates strongly correlates with t'/t, where t' is the second nearest-neighbor hopping amplitude. This contradicts with previous results[12, 13] of exact calculations that for the hole doped systems, introducing t' into the t-J model will actually reduce pairing. Although the last results are studied for systems doped only with a few number of holes, all these conflicting results raised a very serious challenge to the $t-J$ type models.

There are many experimental and theoretical results to support the presence of t' and possibly also t'', the third nearest neighbor hopping, in cuprates. The topology of large Fermi surface seen by ARPES[14, 15] and the change of sign of Hall coefficient as a function of doping[16] can best be understood in the presence of t' and t''. The single hole dispersion observed by ARPES and the difference between hole- and electron-doped systems[17] also support the presence of these terms.

In this letter, we will use variational approach supplemented by slave-boson mean-field (MF) calculations and exact diagonalization (ED) method to show that the presence of t' is indeed important for enhancing pairing beyond the underdoped regime. The largest values of pairing correlation obtained are proportional to t'/t up to $t'/t=-0.3\sim-0.4$. In addition we will show that the decrease of pairing correlation at very large hole density is related to the change of Fermi surface topology. The conflicting results between theories and experiments discussed above are naturally resolved within the extended $t-J$ model.

The Hamiltonian of the extended $t-J$ model is

$$H = H_t + H_J = \tag{1}$$
$$-\sum_{ij} t_{ij}(\tilde{c}^\dagger_{i,\sigma}\tilde{c}_{j,\sigma} + H.C.) + J\sum_{<i,j>}(\mathbf{S_i}\cdot\mathbf{S_j} + \frac{1}{4}n_i n_j)$$

where $t_{ij}=t$, t', and t'' for sites i and j are nearest, next nearest, and the third nearest neighbors, respectively, and $t_{ij}=0$ for longer distance. $\tilde{c}_{i,\sigma}=(1-n_{i,-\sigma})c_{i,\sigma}$, satisfies the no-double-occupancy constraint. In our notation for hole doped materials, t'/t is negative while $t''=-t'/2$ most of the time.

The trial wave function (TWF) used in this study is the $d_{x^2-y^2}$ resonating-valence-bond wave function

$$\mid\Psi\rangle = P_G\prod_k(u_k + v_k c^\dagger_{k,\uparrow}c^\dagger_{-k,\downarrow})\mid 0\rangle \tag{2}$$

with $u_k/v_k=\Delta_k/(\epsilon_k+\sqrt{\epsilon_k^2+\Delta_k^2})$, $\epsilon_k=-2t(cosk_x+cosk_y)-4t'_v cosk_x cosk_y-2t''_v(cos2k_x+cos2k_y)-\mu$, and $\Delta_k=2\Delta(cosk_x-cosk_y)$. Here the projection operator P_G enforces the constraint of one electron per site. In addition to Δ and μ, we have included two important variational parameters t'_v and t''_v which determine the Fermi surface topology.

The d-wave pair-pair correlation $P_d(\mathbf{R})$ is defined as $\frac{1}{N_s}\langle\sum_i \Delta^\dagger_{\mathbf{R_i}}\Delta_{\mathbf{R_i}+\mathbf{R}}\rangle$, where $\Delta_{\mathbf{R_i}}=c_{\mathbf{R_i}\uparrow}(c_{\mathbf{R_i}+\hat{\mathbf{x}}\downarrow}+c_{\mathbf{R_i}-\hat{\mathbf{x}}\downarrow}-c_{\mathbf{R_i}+\hat{\mathbf{y}}\downarrow}-c_{\mathbf{R_i}-\hat{\mathbf{y}}\downarrow})$. The long range part of $P_d(\mathbf{R})$ is a flat plateau for nonzero Δ, and we define P_d^{ave} as the averaged value of the $\mid\mathbf{R}\mid>2$ part of $P_d(\mathbf{R})$ to estimate the strength of SC of the system.

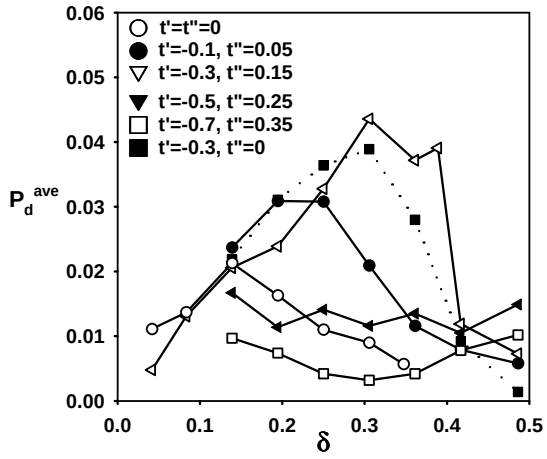

FIG. 1: P_d^{ave} for $J/t = 0.3$ with several t' and t'' for a hole-doped 12×12 lattice.

Fig.1 shows the variational Monte Carlo (VMC) results of P_d^{ave} for several t' and t'' for different hole densities δ with $J/t = 0.3$ in a 12×12 lattice. P_d^{ave} for the $t-J$ model (open circles) has the "dome-like" shape which is similar to the experimental results of T_c versus doping. However, this could be an artifact of the variational study which, we believe, overestimates the order parameters and will be largely suppressed when we go beyond variational calculation as shown in our previous study[5]. The most suprising result is that when t' is included, P_d^{ave} changes dramatically. For the overdoped regime, P_d^{ave} is greatly enhanced by almost one order of magnitude for $t'/t = -0.3$ and $t''/t = 0.15$. The SC region extends to $\delta \sim 0.4$ and the peak of the superconducting dome is at $\delta \sim 0.3$ and the magnitude of the maximal P_d^{ave} is about 2.5 times larger than for $t' = t'' = 0$. In the underdoped region, P_d^{ave} is almost unchanged or very slightly suppressed. Another thing to note is that beyond the value of $t'/t = -0.3 \sim -0.4$ P_d^{ave} is no longer enhanced.

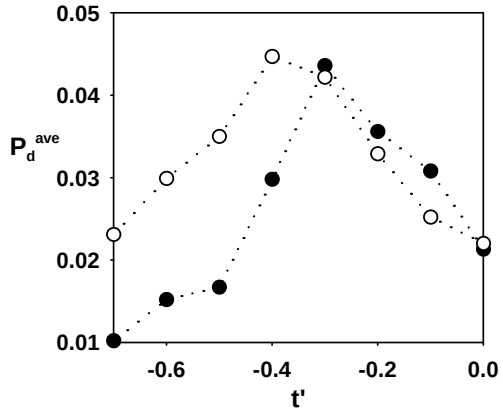

FIG. 2: Maximal P_d^{ave} for different t' with $t'' = -t'/2$ for 8×8 (open circle) and 12×12 (full circle) lattices.

Fig.2 plots the maximal possible value of P_d^{ave} for all doping density as a function of t'. The maximal P_d^{ave} is proportional to t' in the range $0 \geq t' \geq -0.3 \sim -0.4$. Beyond these values pairing is no longer enhanced. Coincidentally these values are about the same value of t'/t for mercury cuprates as estimated by Pavarini *et al.*[10] but much larger than what was reported in Ref.[9]. Among all the cuprate series, mecury cuprate maintains the record of having highest T_c for almost a decade.

The above result resolves the discrepancy between previous denisty-matrix-renormalization-group (DMRG) studies [12, 13] and the band structure calculation [10]. As DMRG studies were concerned with underdoped region while the highest $T_{c,max}$ examined by the band structure calculation certainly depends on optimal and overdoped regions.

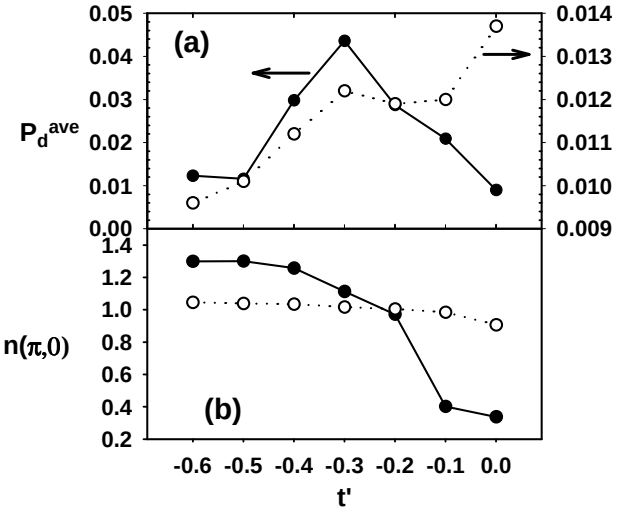

FIG. 3: (a)P_d^{ave} and (b) $n(\mathbf{k} = (\pi, 0))$ vs. t' for $\delta = 0.31$ (full circles) and 0.083 (open circles), $J/t = 0.3$, $t'' = -t'/2$.

The different effects of t' and t'' on P_d^{ave} between overdoped and underdoped regions are related to the shape of Fermi surface. Fig.3 shows the relations of P_d^{ave} and $n(\mathbf{k} = (\pi, 0))$ versus t' for $\delta = 0.31$ and 0.083. For the overdoped case ($\delta = 0.31$), as $-t'$ increases up to 0.3, $n(\mathbf{k} = (\pi, 0))$ increases from less than 0.4 to larger than 1 and P_d^{ave} also increases sharply from less than 0.01 to larger then 0.04. Since $d-$wave SC gap is largest at $\mathbf{k} = (\pi, 0)$, occupation of this $\mathbf{k}$ states by electrons enhances P_d^{ave} . On the other hand for the underdoped case, $n(\mathbf{k} = (\pi, 0))$ is almost unchanged because the occupation $n(\mathbf{k} = (\pi, 0))$ is already quite large (> 0.9) for $t' = t'' = 0$ and the effect of Fermi surface becomes unimportant. The slight suppression of P_d^{ave} may be due to the destructive interference mechanism of the pair-hopping as suggested by Martins *et al.*[13].

The decrease of P_d^{ave} for $-t' \geq 0.4$ in the overdoped regime such as $\delta = 0.31$ is also likely the consequence of the change of the Fermi surface. $n(\mathbf{k} = (\pi, 0))$ is al-

most saturated at $-t' = 0.4$ and remains unchanged for larger $-t'$. It is not difficult to recognize that as $-t'$ becomes much larger than t, electrons will occupy in separate regions around $\mathbf{k} = (\pm\pi, 0)$ and $\mathbf{k} = (0, \pm\pi)$. Hence the Fermi surface becomes disjoint pieces. Although at $-t'/t = 0.4$, the Fermi surface is still connected but this tendency is already observed. The density of states begins to decrease and this is probably the reason for the suppression of pairing beyond $-t'/t' \geq 0.4$.

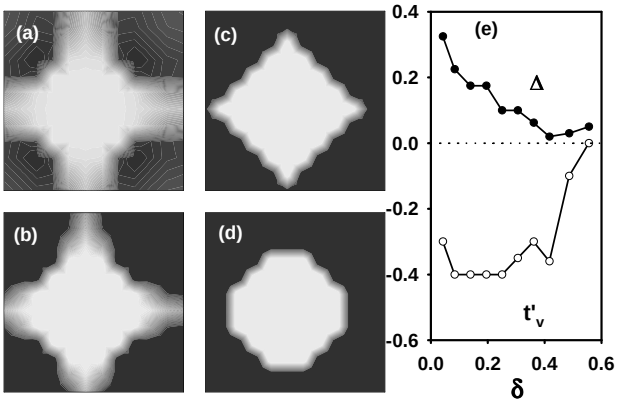

FIG. 4: Fermi surface of $\delta =$ (a)0.19, (b)0.31 (c)0.42 (d) 0.49 for 12×12 lattice. (e)optimal parameters t'_v (squares) and Δ (circles).

Fig.4 shows the Fermi surface and optimal parameters Δ and t'_v as a function of doping density for a 12×12 lattice with $J/t = 0.3$, $t' = -0.3$ and $t'' = 0$. In (a-d) the white region denotes $n(\mathbf{k}) \geq 1.2$ and dark region for $n(\mathbf{k}) \leq 0.5$. The density with maximal P_d^{ave} is near $\delta_{opt} = 0.31$ as shown by the solid square in Fig.1. The shapes of the Fermi surfaces are very different for $\delta > \delta_{opt}$ and $\delta < \delta_{opt}$ cases. Fig.4(e) shows that in the region $0.2 < \delta < 0.3$ although Δ becomes smaller, $-t'_v$ is still quite large and pairing is further enhanced. Doping beyond $\delta > 0.3$, $-t'_v$ begins to decrease quickly. This gives very low electron occupation at $(\pi, 0)$ as shown in Fig.4(c) and (d), then the pairing is reduced. This result shows that the enhancement of pairing by including t' is not due to larger Δ but from the deformation of the Fermi surface instead.

Although we have emphasized the particular correlation between d-wave SC gap and electron occupation at $\mathbf{k} = (\pi, 0)$ as the reason for enhancement of pairing, another familiar effect may also have played a role. It is well known that t' will shift the van Hove singularity[18] in density of states, but it is always around $\mathbf{k} = (\pi, 0)$. Hence it could be that the optimal t'_v are chosen to have the high density of states at Fermi surface. This may be related to the observed extended region of flat band by ARPES[19].

The results of slave-boson MF calculation[20] in Fig.5 show similar behavior for the overdoped regime that indeed t' enhances T_c. Including t'' pushes the superconducting regime to even larger doping density δ by occupying the momenta around $(\pi, 0)$. A similar effect of t'' can also be seen in Fig.1 by comparing the $(t', t'') = (-0.3, 0)$ (full squares) and $(-0.3, 0.15)$ (open triangles) curves. Since the slave-boson method is not quite reliable quantitatively in the underdoped regime, we did not show the values of T_c in Fig.5. However, if we do take the values literally, the values achieved for $T_{c,max}$ are not as greatly enhanced by t' as for the VMC result shown in Fig.2. Similar results are reported by the interlayer tunneling model[21].

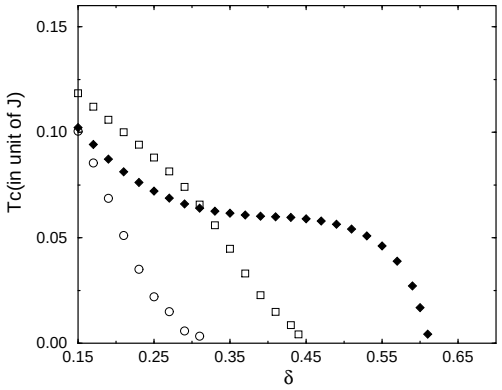

FIG. 5: Mean-field results of T_c for overdoped regime with $(t', t'') = (0, 0)$ (circles), $(-0.3, 0)$ (squares) and $(-0.3, 0.15)$ (diamonds).

Fig.6 shows the pair-pair correlation[22] for the longest distance $\mathbf{R} = (1, 3)$ for 20-site lattices obtained by the ED method. Pairing correlations for 2 and 4 holes are suppressed by t' and t'', but enhanced for the overdoped 6- and 8-hole cases. The non-monotonic behavior of the overdoped cases is due to the level crossing of this system. If we focus on the $s-$like symmetry states, P_d^{ave} will vary monotonically in the region $0 \geq t' \geq -0.3$. The result of ED method is quite consistent with the variational and MF results that the enhancement of P_d^{ave} by t' occurs for larger hole densities.

In summary, in the optimal and overdoped regions, SC is greatly enhanced because of the deformation of the Fermi surface at these doping densities. $n(\mathbf{k} = (\pi, 0))$ is enhanced by including t' and t''. The occupation of $(\pi, 0)$ by electrons is important for the enhancement. The maximum enhancement of pairing correlation seems to be reached for $-t'/t = 0.3 \sim 0.4$. On the other hand, P_d^{ave} is not enhanced for the underdoped regime as $n(\mathbf{k} = (\pi, 0))$ is hardly affected by including t'. It is well accepted that the physics on the overdoped side is apparently much simpler in that experiments on the cuprates and theory for the t-J model indicate that the overdoped materials are very close to ordinary Fermi liquids, whence 'Fermi-

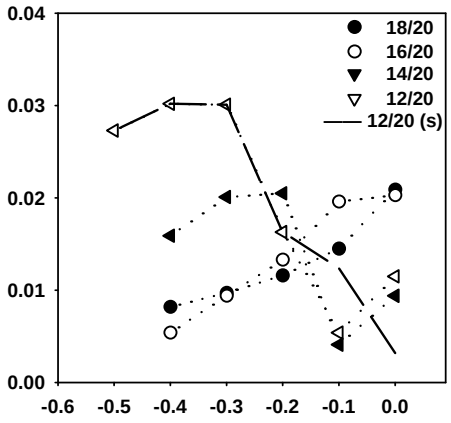

FIG. 6: $P_d(\mathbf{R}=(1,3))$ for versus t' ($t''=-t'/2$) for different 2 (open circle) , 4 (full circle), and 6 (open triangle) holes in 20 sites. The dash line shows P_d for the same symmetry of the 8-hole case.

surface-based' arguments like ours are much more reliable than in the underdoped region. Our result shows that the extended $t-J$ model naturally predicts the strong correlation[10] between t'/t and $T_{c,max}$ observed in experiments for monolayer cuprates. In addition it also indicates that further increase of t' beyond what mercury cuprates have most likely will not enhance $T_{c,max}$.

Although we have consistent results from VMC, ED methods and slave-boson MF calculations, the optimal doping density, δ_{opt}, in Fig.1 is around 0.3 instead of 0.17 obtained in the experiments and in the VMC results without including t'. But this is actually not a drawback. As argued in References[5, 7], VMC is expected to overestimate the values of the variational parameters Δ which is related to the exhange energy J. Hence the pairing correlation is definitely much larger than that of a real ground state. From our previous experiences the δ_{opt} seems to be always shifted to a smaller value when we improve the variational wave functions. Thus in the future work going beyond VMC calculations, we believe there is a better chance that we will have δ_{opt} closer to the experimental value. We also expect interlayer coupling will be important in getting the correct δ_{opt}. Now t' is shown to be important in enhancing pairing and it is also present in all high T_c cuprates, the debate[7, 8] about pairing robustness in the 2D $t-J$ model without t' becomes somewhat irrelevant. The agreement of δ_{opt} between $t-J$ VMC and experiments looks fortuitous.

One of the consequences of our results is that the shape of the Fermi surface plays an important role for high temerature superconductors in the optimal and overdoped regions. Fig.4 (b) and (c) show that the Fermi surface changes from hole-like to electron-like once the maximum pairing is reached and the pairing is reduced as doping increases. This is consistent with the ARPES results for $La_{2-x}Sr_xCuO_4$[15]. It may also be related to the recent experiment[23] which shows that the low-temperature Hall coefficient for the $Bi_2Sr_{1.51}La_{0.49}CuO_{6+\delta}$ system exhibits a sharp change at the optimal doping density. Clearly this issue deserves more detailed study in the future.

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